

Integrability and Computability in Simulating Quantum Systems

K. Umeno*

Laboratory for Information Representation, Frontier Research Program
The Institute of Physical and Chemical Research (RIKEN)
2-1 Hirosawa, Wako, Saitama 351-01, Japan

Abstract

An impossibility theorem on approximately simulating quantum non-integrable Hamiltonian systems is presented here. This result shows that there is a trade-off between the unitary property and the energy expectation conservation law in time-discretization of quantum non-integrable systems, whose classical counterpart is Ge-Marsden's impossibility result about simulating classically non-integrable Hamiltonian systems using integration schemes preserving symplectic (Lie-Poisson) property.

1 Introduction

Recently, much attentions are directed to investigate the interrelation between physics and computation. To connect physics with computation, we can classify the problems into the the following classes:

- class (1): Connection between classical physics and classical computation,
- class (2): Connection between quantum physics and classical computation,
- class (3): Connection between classical physics and quantum computation, and
- class (4): Connection between quantum physics and quantum computation.

Concerning the class (4), *simulating* quantum behavior such as quantum chaos using classical computers is known to be a notoriously difficult computational problem[4]. One

*E-mail: chaosken@giraffe.riken.go.jp

of the main difficulties is that one must discretize a continuous time parameter of equations of motion in order to simulate on computers. Thus, it is an important question to ask whether we can always have a suitable time-discretization scheme of Schrödinger equation.

In this paper, I will give a somewhat negative answer to this question: In the case of *quantum non-integrable* systems with an explicit time-independent Hamiltonian operator, no *explicit* time-discretization algorithm preserving unitary property can simulate quantum non-integrable behavior without violating the conservation law of energy expectation. Since the original quantum nature must have these two properties, namely, the conservation law of energy expectation and the unitary property of time evolution, this means that there is a fundamental limit in simulating quantum non-integrable behavior using unitary maps like quantum computers. This negative result can be regarded as a quantum analogue of Ge-Marsden's theorem[7]: No symplectic integrator can simulate non-integrable behavior in a class of autonomous Hamiltonian systems without violating the energy conservation. These fundamental limits, whether quantum or classical, suggest the importance of the notion of integrability in simulating physical behavior. In Section 2, we give a brief explanation of time-discretization preserving unitary property. In Section 3, we give a theorem about the impossibility of simulating quantum non-integrable systems. In Section 4, we discuss various aspects about our results.

2 Simulation technology preserving unitary property

Time-evolution of quantum computation can be seen as a class of successive iterations of unitary transformations[1, 2, 5]. The time-evolution operator has the form of

$$U(\Delta t) = \exp [-i\Delta t H/\hbar], \quad (1)$$

where H is a Hamiltonian operator with Hermitian property, Δt is the time duration of each computation process and an exponential operator $\exp [xA]$ is defined as

$$\exp [xA] = \sum_{n=0}^{\infty} \frac{(xA)^n}{n!}, \quad x = -i\Delta t/\hbar. \quad (2)$$

Let A and B be Hermitian operators as the generators of two *different* elementary processes of unitary dynamics. In general, A does not commute with B :

$$[A, B] = AB - BA \neq 0. \quad (3)$$

To track computational processes retaining unitary property, evaluating the following time-evolution operator

$$\exp [x(A + B)] \quad (4)$$

is relevant to various problems. In fact, there are infinitely many methods to get perturbation series of Eq.(4). The Feynman path-integral method[3]

$$\exp [x(A + B)] \approx \left[1 + \frac{x(A + B)}{n} \right]^n \quad (5)$$

discovered in his study of quantum electro-dynamics is a first-order method based on the identity

$$\exp [x(A + B)] = \lim_{n \rightarrow \infty} \left[1 + \frac{x(A + B)}{n} \right]^n. \quad (6)$$

However, the above approximation breaks unitary property in each elementary dynamical process $1 + \frac{x(A+B)}{n}$, as is easily checked. On the contrary, Trotter formula [14]

$$\exp [x(A + B)] = \left[\exp\left(\frac{xA}{n}\right) \exp\left(\frac{xB}{n}\right) \right]^n + O\left(\frac{x^2}{n}\right) \quad (7)$$

based on the identity

$$\exp [x(A + B)] = \lim_{n \rightarrow \infty} \left[\exp\left(\frac{xA}{n}\right) \exp\left(\frac{xB}{n}\right) \right]^n \quad (8)$$

preserves the unitary property in each elementary process $\exp(\frac{xA}{n}) \exp(\frac{xB}{n})$, as is also easily checked. The second order formula called Leap flog method has the form

$$\exp [x(A + B)] = \left[\exp\left(\frac{xA}{2n}\right) \exp\left(\frac{xB}{n}\right) \exp\left(\frac{xA}{2n}\right) \right]^n + O\left(\frac{x^3}{n^2}\right). \quad (9)$$

Furthermore, many other higher-order formulas for exponential operators $\exp [x(A + B)]$ preserving the symmetry corresponding to the unitary property were recently discovered independently both in the development of simulation technology called quantum Monte Carlo methods [10, 13] to simulate density matrices, or in the development of simulation technology called symplectic integrators [9, 11, 12, 13, 15, 23] to simulate classical Hamiltonian dynamical systems. It is an easy task to extend these decomposition formula of the exponential operators $\exp [x(A + B)]$ to more generalized exponential operators $\exp [x \sum_{j=1}^l A_j]$ of multi noncommutative operators A_1, A_2, \dots, A_l . Thus, an application of these successive composition formulas of exponential operators to quantum computations of $\exp [x \sum_{j=1}^l A_j]$ can give us a unified view of this kind of simulations as follows: Let us consider the problem of approximately simulating $\exp [x \sum_{j=1}^l A_j]$ for $t \leq t' \leq t + \Delta t$ based on an explicit algorithm on quantum model of computation whose

each elementary process is successively generated by explicitly time-dependent Hamiltonians $Q_j(t, \Delta t)$, $1 \leq j \leq m$. Then, each s -th order approximation formula has a form:

$$\exp \left[x \sum_{j=1}^l A_j \right] = \prod_{j=1}^m \exp [x Q_j(t, \Delta t)] + O(x^{s+1}). \quad (10)$$

The relation

$$\sum_{j=1}^l A_j = \sum_{j=1}^m Q_j(t, \Delta t) \quad (11)$$

must hold from the lowest order terms in x in Eq. (10).

3 Theorem

Let us consider a time-independent Hamiltonian $H(\mathbf{q}, \mathbf{p})$ in a certain class of the set of Hermitian operators $\tilde{G} = \{G(\mathbf{q}, \mathbf{p})\}$, where \mathbf{q} and \mathbf{p} denotes the canonical conjugate operators in the standard sense of quantum mechanics. We can define *quantum non-integrability* as follows:

Definition 1 *We call a quantum Hamiltonian system with a time-independent Hamiltonian operator H quantum non-integrable if the following relation holds:*

$$[\Phi, H] = 0 \implies \Phi = F(H), \quad (12)$$

where $\Phi \in \tilde{G}$ and F is a some function of a variable.

Since H is a time-independent Hamiltonian operator, the expectation value of H must be preserved:

$$\frac{d}{dt} \langle H \rangle = \frac{d}{dt} \langle \Psi | H | \Psi \rangle = 0, \quad (13)$$

where $\langle \Psi |$ is the state vector.

Here, we prove the following theorem:

Theorem 1 *If an explicit algorithm preserving unitary property can simulate a quantum non-integrable system with a time-independent Hamiltonian H approximately, the conservation law of the expectation value of the Hamiltonian operator $\langle H \rangle$ must break down.*

Remark 1: This theorem does *not depend* on the order and types of approximate algorithms we choose.

Remark 2: A class of explicit algorithms preserving unitary property involves universal quantum Turing machines in the sense of Deutsch[2]. Thus, as is shown in Ref. [19, 20], this theorem shows that there is no (discrete time) quantum computers to simulate quantum non-integrable systems without breaking the conservation law of the energy expectation. However, the present theorem says not only the limitation of quantum computers on this aspect but also a more general statement that there is a universal trade-off between the unitary property and the conservation law of energy expectation in time-discretization of quantum non-integrable systems.

(Proof of Theorem 1)

By using the expression of quantum algorithms in Eq. (10), we can consider an s -th order algorithm of approximately simulating the quantum dynamics of H for the time duration Δt of a computational step as follows:

$$\exp[xH] = \prod_{j=1}^m \exp[xQ_j(t, \Delta t)] + O(x^{s+1}), \quad (14)$$

where $x = -i\Delta t/\hbar$ and $1 \leq s < \infty$. Each quantum algorithm $Q_j(t, \Delta t)$ has a corresponding *time-dependent* Hamiltonian $H_j(t)$ satisfying

$$Q_j(t, \Delta t) = T(\exp \int_t^{t+\Delta t} H_j(s) ds) = 1 + \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_0^{t_1} dt_1 \cdots \int_0^{t_{n-1}} dt_n H_j(t_1) \cdots H_j(t_n), \quad (15)$$

where T denotes the time ordering. The resulting quantum algorithm has also an *time-dependent* Hamiltonian $\tilde{H}(t, \Delta t)$ satisfying the relation

$$\prod_{j=1}^m \exp[xQ_j(\Delta, t)] = \exp(x\tilde{H}(t, \Delta t)). \quad (16)$$

By successively applying the Baker-Campbell-Hausdorff formula:

$$\exp X \exp Y = \exp Z, \quad (17)$$

where

$$Z = X + Y + \frac{1}{2}[X, Y] + \frac{1}{12}([X, [X, Y]] + [Y, [Y, X]]) + \frac{1}{24}[X, [Y, [Y, X]]] + \cdots \quad (18)$$

to the system (16), we can compute the corresponding time-dependent Hamiltonian \tilde{H} in a form:

$$\tilde{H}(\mathbf{q}, \mathbf{p}, t, \Delta t) = H + \sum_{n=s}^{\infty} (\Delta t)^s H_s(t) = H + O(x^s), \quad (19)$$

where $H_s(t)$ is a time-dependent correction term of order s . We assume that the energy expectation $\langle \tilde{H} \rangle$ in the quantum simulation is also preserved:

$$\langle H \rangle = \langle \tilde{H} \rangle = \text{Const.} \quad \text{for } t \leq t' \leq t + \Delta t. \quad (20)$$

Since we can choose Δt an arbitrary real number, the relation (20) means the following commutation relations hold:

$$[H, \tilde{H}(t)] = 0 \quad \text{and} \quad [H, H_n(t)] = 0 \quad \text{for } n \geq s. \quad (21)$$

However, from the assumption of *quantum non-integrability* of H , it follows that that $\tilde{H} = F(H)$. This means that the quantum algorithm \tilde{H} generates the *exact* quantum dynamics of H . This exactness ($s \rightarrow \infty$) contradicts the assumption that the underlying quantum algorithm gives an *approximate* tracking of the dynamics of H in the finite order s .

(End of Proof)

4 Discussions

The key of the present analysis is in *quantum non-integrability*. How generic is the notion of quantum non-integrability in quantum mechanics? In classical mechanics, it is known that most dynamical systems are non-integrable since the famous Poincaré theorem in the last century. Furthermore, we have exact criteria of classical non-integrability for explicitly given Hamiltonian systems based on the singularity analysis [8, 16, 17, 18, 22, 24, 25].

On the contrary, in quantum mechanics, we do not have any theorem guaranteeing the generic character of quantum non-integrable systems corresponding to the Poincaré theorem in classical mechanics nor exact criteria of quantum non-integrability for explicitly given Hamiltonian operators. In other words, it is not a trivial thing to connect classical non-integrability with quantum non-integrability [6, 21]. Recently, the present author found that the quantum Hamiltonian system with a time-independent Hamiltonian operator $H = \frac{1}{2}(p_x^2 + p_y^2 + q_1^2 q_2^2)$ would be quantum-nonintegrable under the hypothesis of the Weyl rule for canonical variables p_i, q_i using the Moyal bracket, based on Ziglin's result of proof of its classical non-integrability [20]. For the classical system of this system, it was shown in Ref. [15] that we cannot avoid energy fluctuations for some specific initial conditions like $(q_1, q_2, p_1, p_2 = (1000, 0.002, 0, 0))$ because the higher-order correction terms H_s also become bigger as

$$|H_s| \approx AB^s, \quad (22)$$

where A and B are some positive real constants. It can be easily predicted that this divergence of the higher-order correction terms H_s can also occur in quantum non-integrable

systems like a quantum version of the above system. This model can be a vivid example causing rather general phenomena of the breakdown of the conservation law of energy expectation for quantum non-integrable systems by using any finite-order time-discretization preserving unitary property, which Theorem 1 asserts. This result has an interesting implication concerning the usual energy-time uncertain relations. From the energy-time uncertain relations $\Delta t \cdot \Delta E \geq \hbar$, it follows that

$$\Delta t^s |H_s| \approx \Delta E \geq \frac{\hbar}{\Delta t}. \quad (23)$$

This inequality gives a lower-bound of Δt which depends only on the order s of time-discretization and the correction terms H_s . Thus, this analysis shows that our naive view that the continuous nature of time in quantum mechanics is naturally obtained in the continuum limit $\Delta t \rightarrow 0$ is not universal, at least in quantum non-integrable systems. It will be an interesting and important open problems to consider time-discretization of quantum non-integrable systems in connection with the foundation of quantum mechanics.

Acknowledgements

This work was supported in part by the Special Researcher's Program to promote basic sciences at RIKEN and from the Frontier Research Program. I would like to thank Prof. Shun-ichi Amari for his continual encouragement.

References

- [1] BENIOFF, P., "Quantum mechanical Hamiltonian models of Turing machines," *J. Stat. Phys.* **29** (1982), 515-546.
- [2] DEUTSCH, D., "Quantum theory, the Church-Turing principle and the universal quantum computer," *Proc. R. Soc. Lond. A* **400** (1985), 96-118.
- [3] FEYNMAN, R. P., "An operator calculus having applications in quantum electro-dynamics," *Phys. Rev.* **84** (1951), 108-128.
- [4] FEYNMAN, R. P., "Simulating physics with computers," *Int. J. of Theor. Phys.* **21** (1982), 467-488.
- [5] FEYNMAN, R. P., "Quantum mechanical computers," *Foundations of Physics* **16** (1986), 507-531.
- [6] HIETARINTA, J., "Quantum integrability is not a trivial consequence of classical integrability," *Phys. Lett. A* **93** (1982), 55-57. i

- [7] GE, Z. and J. E. MARSDEN, “Lie-Poisson Hamilton-Jacobi theory and Lie-Poisson integrators,” *Phys. Lett. A* **133** (1988), 134–139.
- [8] ITO, H., “Non-integrability of Hénon-Heiles system and a theorem of Ziglin,” *Kodai Math. J.* **8**(1985), 120-138.
- [9] RUTH, R. D., “A canonical integration technique,” *IEEE Trans. on Nuclear Sci.* **30**(1983), 2669-2671.
- [10] SUZUKI, M.(Editor), *Quantum Monte Carlo Methods*, Springer-Verlag (1987).
- [11] SUZUKI, M., “General theory of higher-order decomposition of exponential operators and symplectic integrators,” *Phys. Lett. A* **165**(1992), 387-395.
- [12] SUZUKI, M., “General decomposition theory of ordered exponentials,” *Proc. Japan. Acad. Ser. B*(1993), 161-166.
- [13] SUZUKI, M. and K. UMENO, “Higher-Order decomposition theory of exponential operators and its applications to QMC and nonlinear dynamics.” In *Computer Simulation Studies in Condensed-Matter Physics VI*, Springer-Verlag (1993), 74-86.
- [14] TROTTER, H. F. *Proc. Am. Math. Phys.* **10** (1959)545.
- [15] UMENO, K. and M. SUZUKI, “Symplectic and intermittent behaviour of Hamiltonian flow,” *Phys. Lett. A* **181** (1993), 387-392.
- [16] UMENO, K., “Non-integrable character of Hamiltonian systems with symmetric and global coupling,” *Physica D* **82** (1995), 11-35.
- [17] UMENO, K., “Non-perturbative non-integrability of non-homogeneous nonlinear lattices induced by non-resonance hypothesis,” *Physica D* **94** (1996), 116-134.
- [18] UMENO, K., “Variational symmetry in non-integrable Hamiltonian systems,” *J. of Nonlinear Mathematical Physics* **4** (1996), (1996), 69-77.
- [19] UMENO, K. “Simulating quantum non-integrable systems with quantum computers”, Extended abstract accepted for Workshop of *PhysComp 96*(1996).
- [20] UMENO, K. “Simulating quantum chaos with quantum computers”, submitted to World Scientific(Singapore), *Proc. of APCTP(Asia Pacific Center for Theoretical Physics) Inauguration Conference* June 4-10(1996) Seoul, Korea.
- [21] WEIGERT, S. “The problem of quantum integrability” *Physica D* **56**(1992)107-119.
- [22] YOSHIDA, H., “A criterion for the non-existence of an additional integral in Hamiltonian systems with a homogeneous potential,” *Physica D* **29** (1987),128-142.

- [23] YOSHIDA, H. “Construction of higher order symplectic integrators,” *Phys. Lett. A***150** (1990), 262-268.
- [24] ZIGLIN, S. L., “Branching of solutions and non-existence of first integrals in Hamiltonian mechanics. I.” *Functional Anal. Appl.***16** (1983), 181-189.
- [25] ZIGLIN, S. L., “Branching of solutions and non-existence of first integrals in Hamiltonian mechanics. II.” *Functional Anal. Appl.***17** (1983), 6-17.